Røntgenlasere – XFELs, hvad de er og hvad de kan

Kristoffer Haldrup, NEXMAP sektionen, DTU Fysik

(og med tak til alle dem jeg har stjålet figurer fra...!)

Centre for Molecular Movies

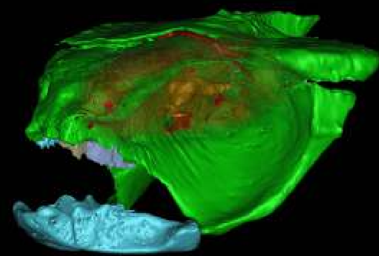
Technical University of Denmark

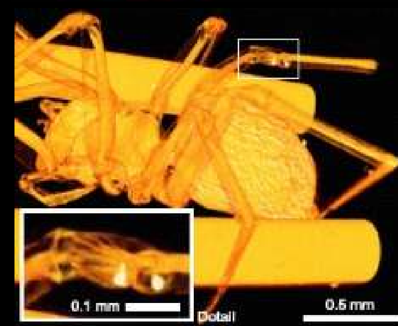
NEXMAP

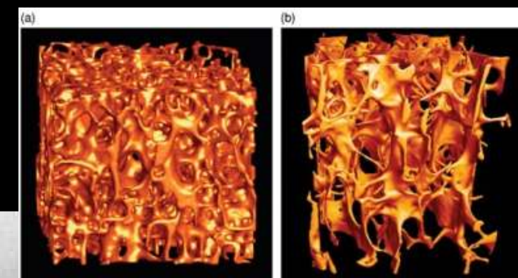
Synkrotron-røntgenstråling er nyttigt...

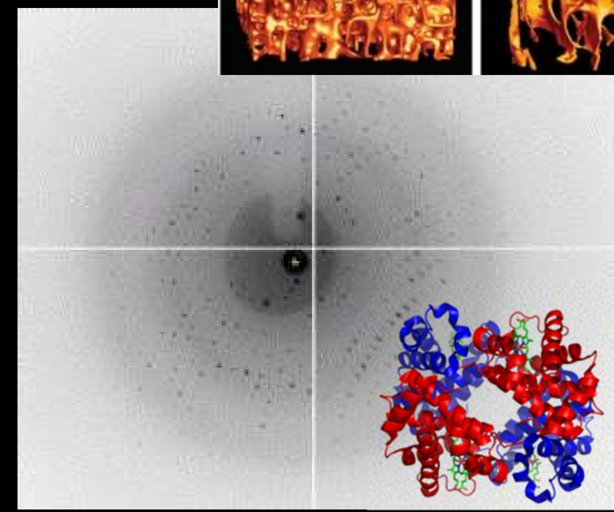
Synktrotron-røntgenstråling kan bruges til "en del":

Fossiler
Krystaller
Knogler
Insekter
Proteiner
Metaller
.
.
.



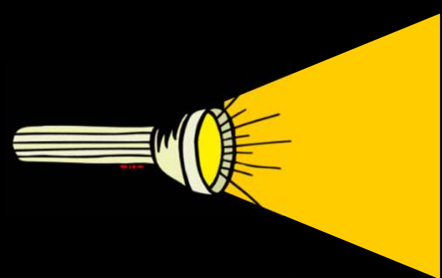






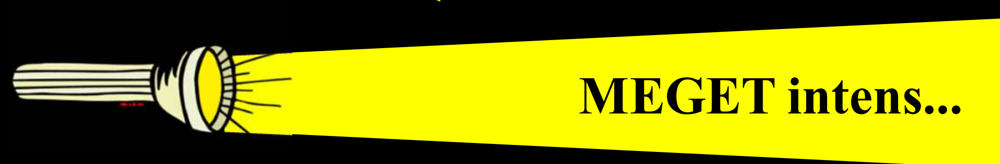
-Men hvad hvis vi kunne gøre det ENDNU bedre?

Afbøjningsmagnet:

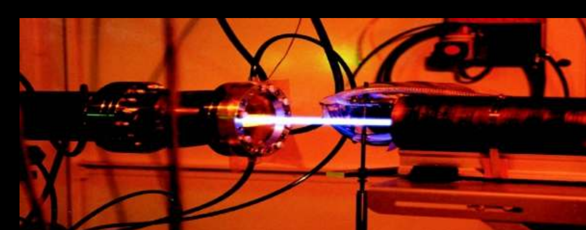


Rimeligt intens...

Insertion device:



100 W/mm^2

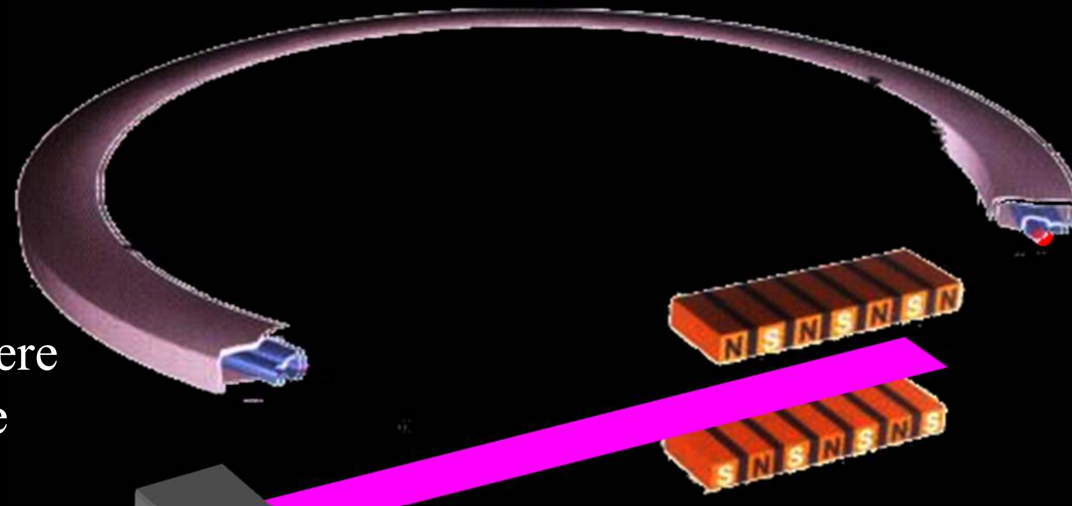


Røntgen-LASEREN er det næste skridt!

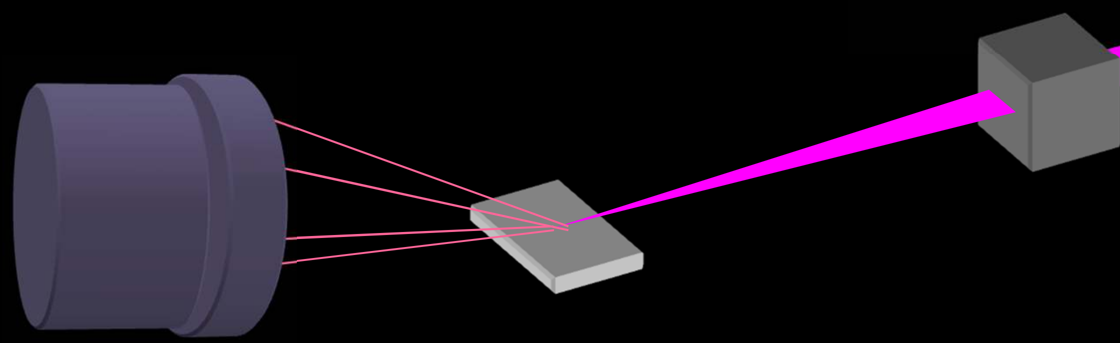
Røntgenstrålelasere, hvad kræver det?

Molecular Movies

I synkrotronerne bliver elektron-bundterne genbrugt over en million gange i sekundet...



Til en røntgen-laser skal elektronbundterne være *ekstra* ”pæne”, så den slags genbrug duer ikke



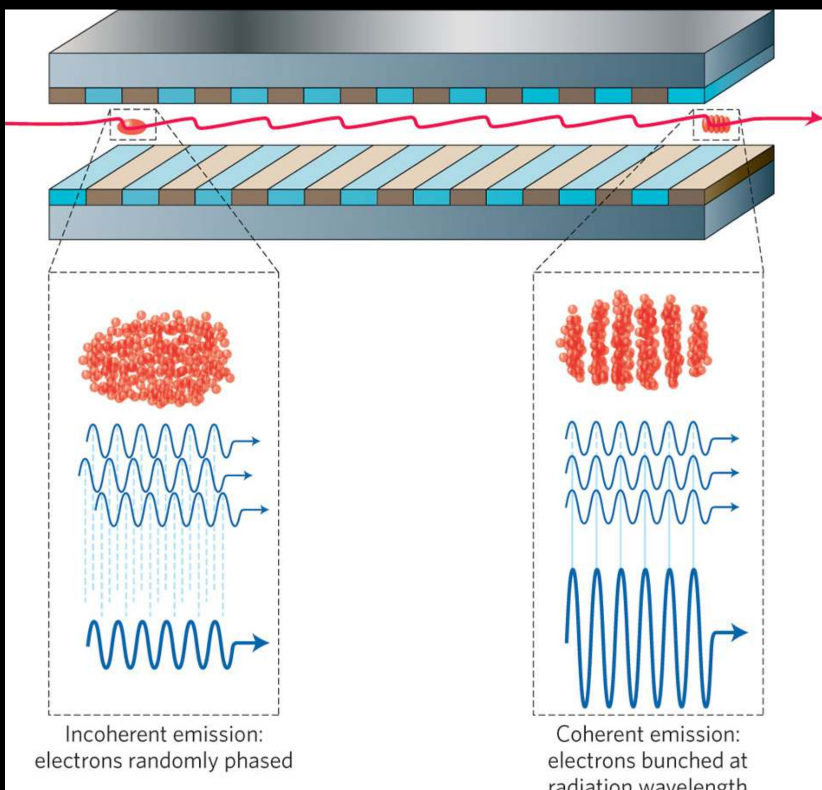
Løsning: ”ret ringen ud”, dvs. byg en LINAC

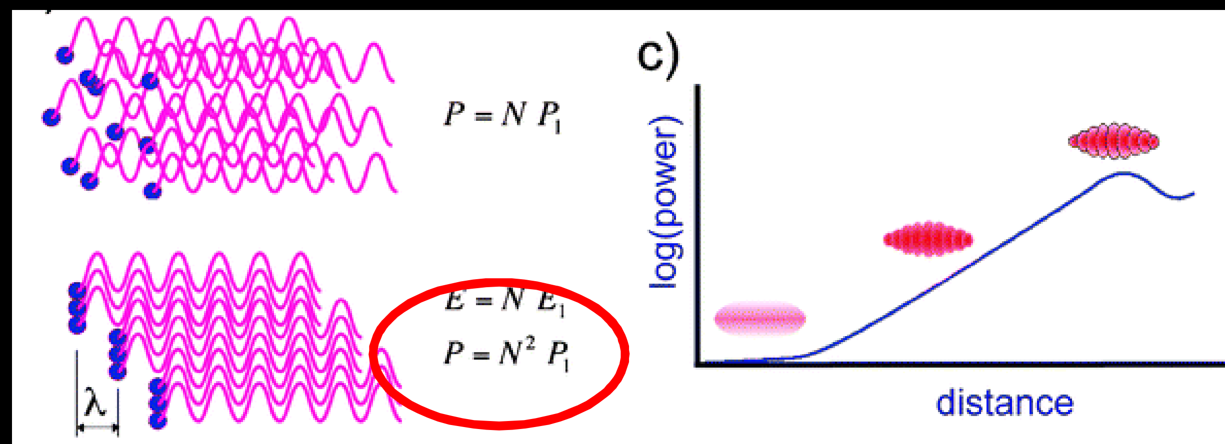
LCLS røntgenlaser ved SLAC, Californien

Meget pæne elektronbundter +
meget lang undulator

=> Elektronbundtet vekselvirker med det udsendte strålingsfelt
⇒ ”micro-bunching”
⇒ SASE, Self-Amplified Spontaneous Emission

~100 meter



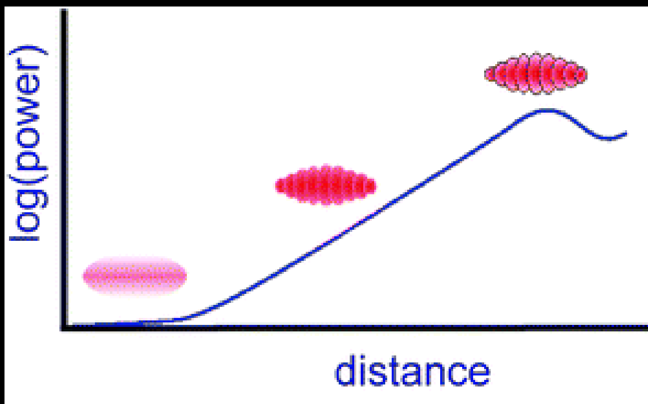


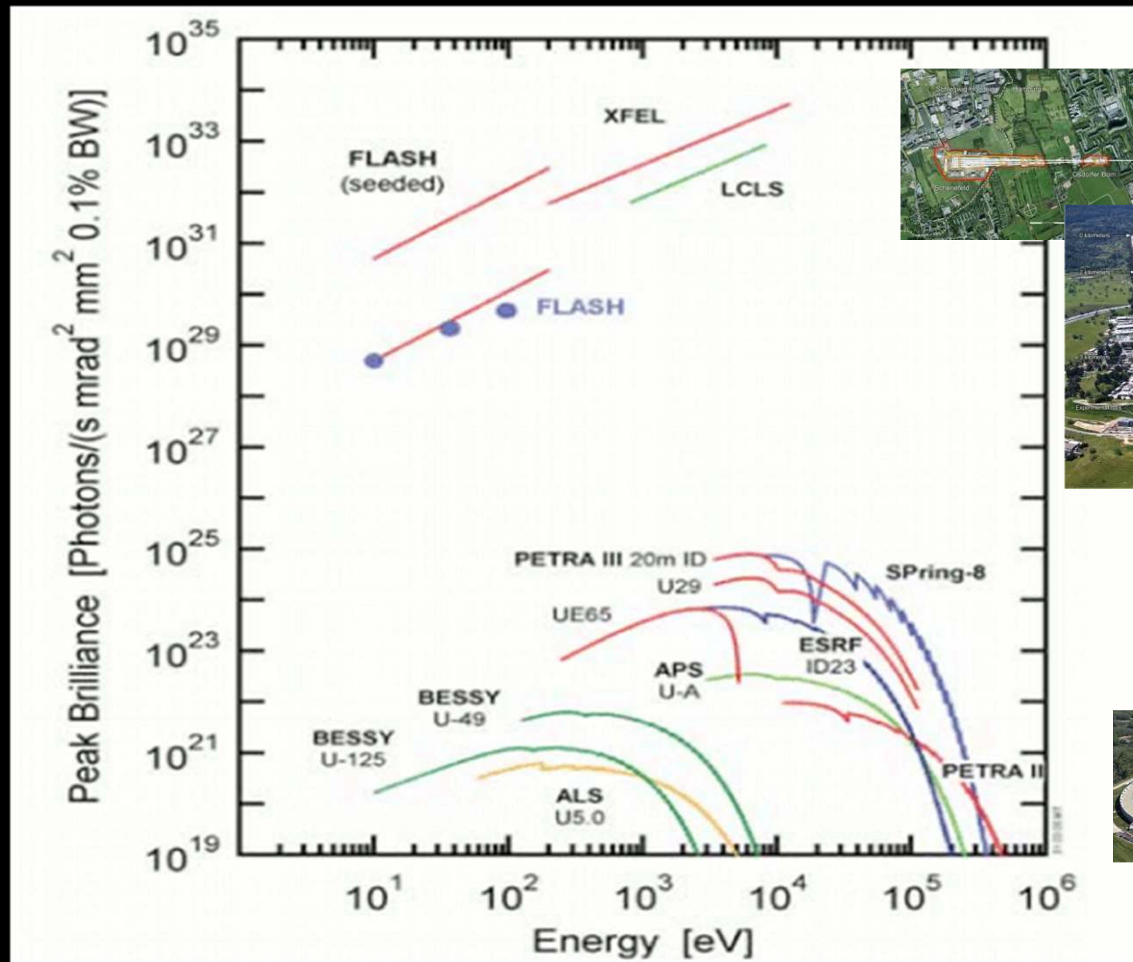
Strålings-effekt proportional med N^2

-og $N \approx 10^9\ e^-$

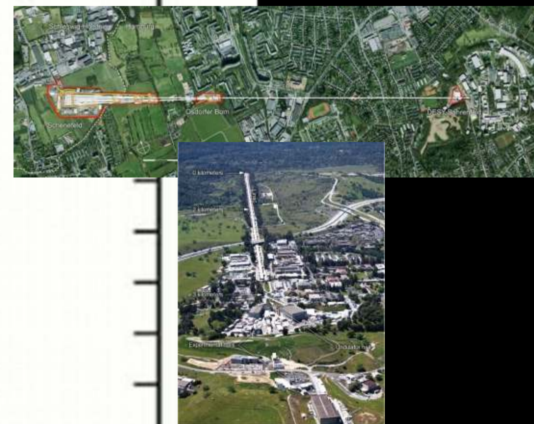
Molecular Movies

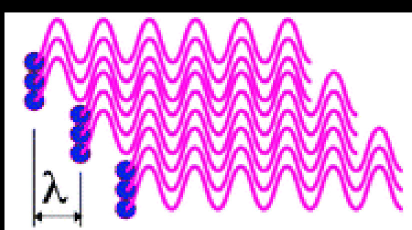
SASE giver ca. 10^6 mere *intense* røntgenpulser...





E-XFEL



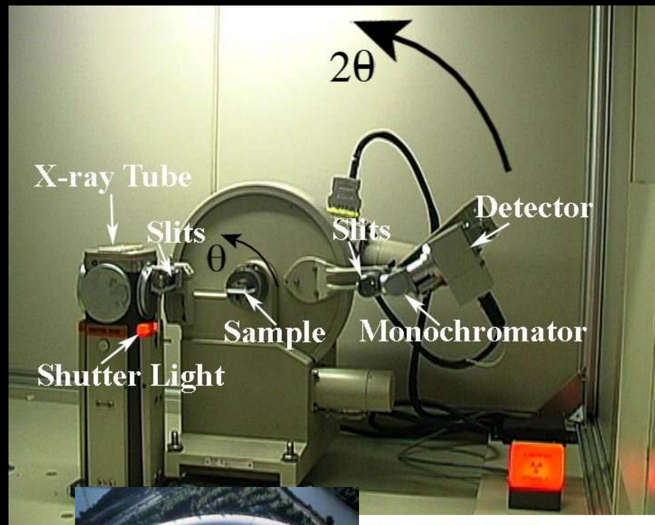


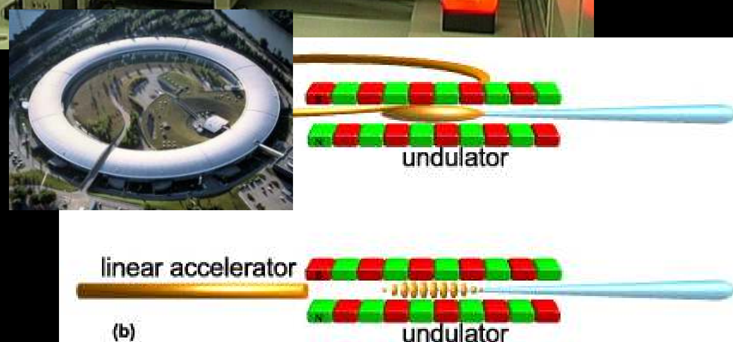
+pulserne er *koherente*, i modsætning til fra synktrotroner, hvor det bare er en (kraftig!) byge af fotoner

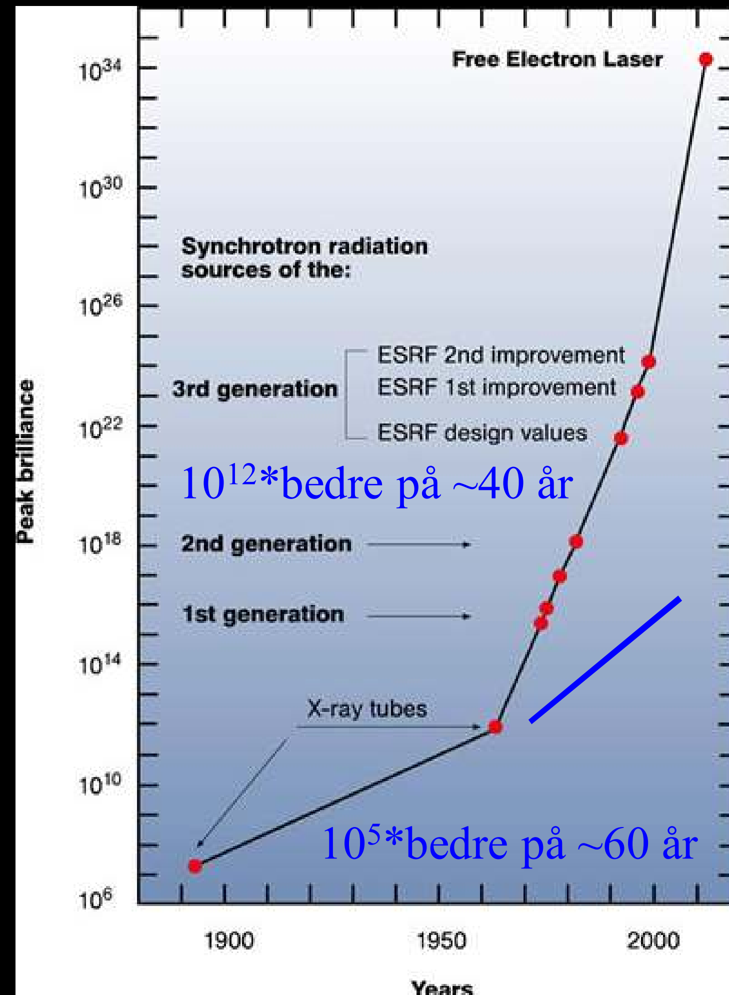
Derfor har maskinerne fået navnet *X-ray Free Electron Lasers* (men, ingen populations-inversion)

Molecular Movies

Sammenligning, røntgenkilder over tid







XFEL parametre:

X-ray energy, 100 eV – 10 keV

X-ray photons/pulse, $\sim 10^{12}$

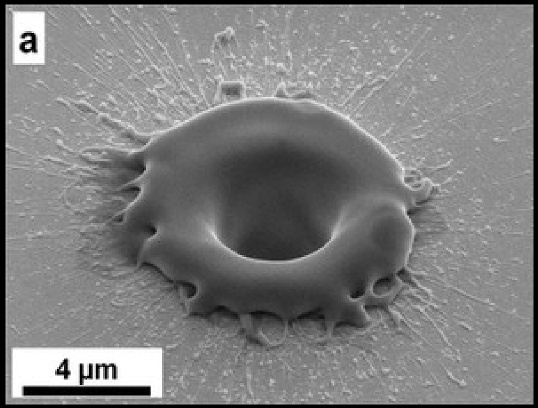
Energy/pulse ~ 1 mJ (10^{12} ph/pulse * $1.602 \cdot 10^{-19}$ J/eV * 10 keV)

Pulse length ~10-100 fs (1 fs = 10^{-15} s, synkrotroner ca. 100 ps = 10^{-10} s)

=> Peak power ~ 1 mJ/10^{-13} s ~ 10 GW

XFEL kilder er....ret intense

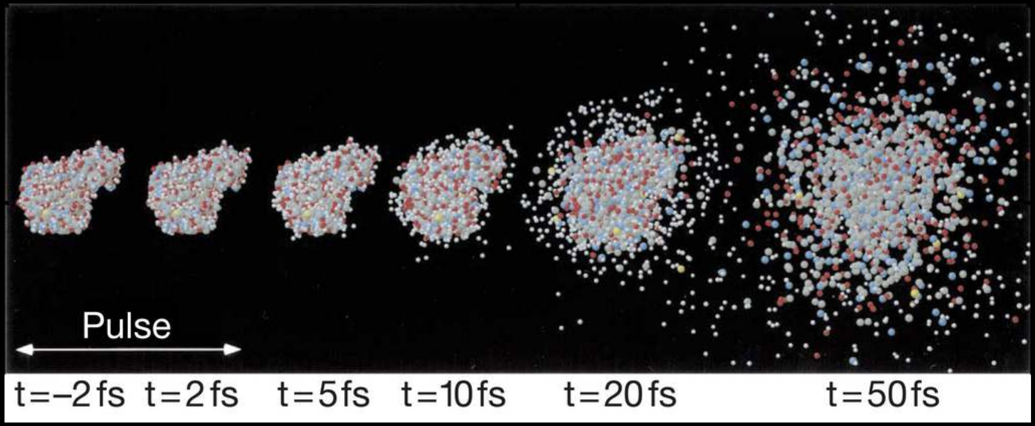
XFEL kilder er....ret intense



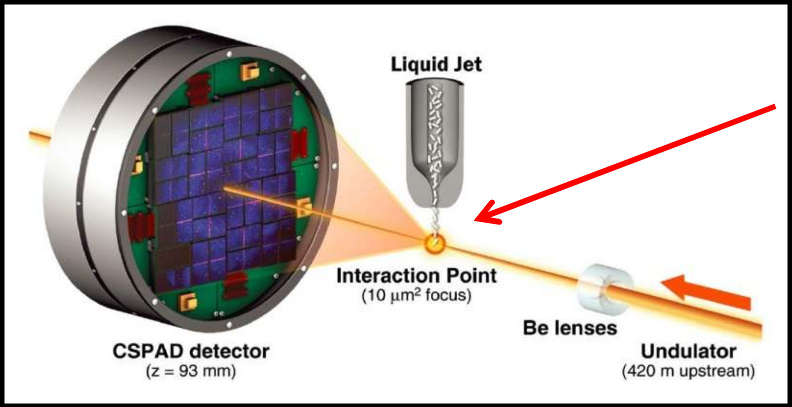
Eet fokuseret skud på Au-dækket glas, 0.05 mJ puls-energi....

1/500.000 af eet nanosekund senere...

Modellering af lysozyme-protein udsat for XFEL-puls:



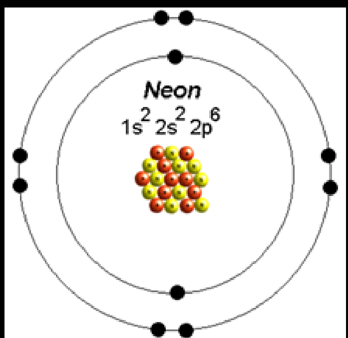
Detektoren har en hul i midten...



-Og prøven bliver skudt igennem røntgenstrålingen

Intensiteten kan bruges til at studere ”Matter in Extreme Conditions”, og til at pille løg fra kernen og ud...

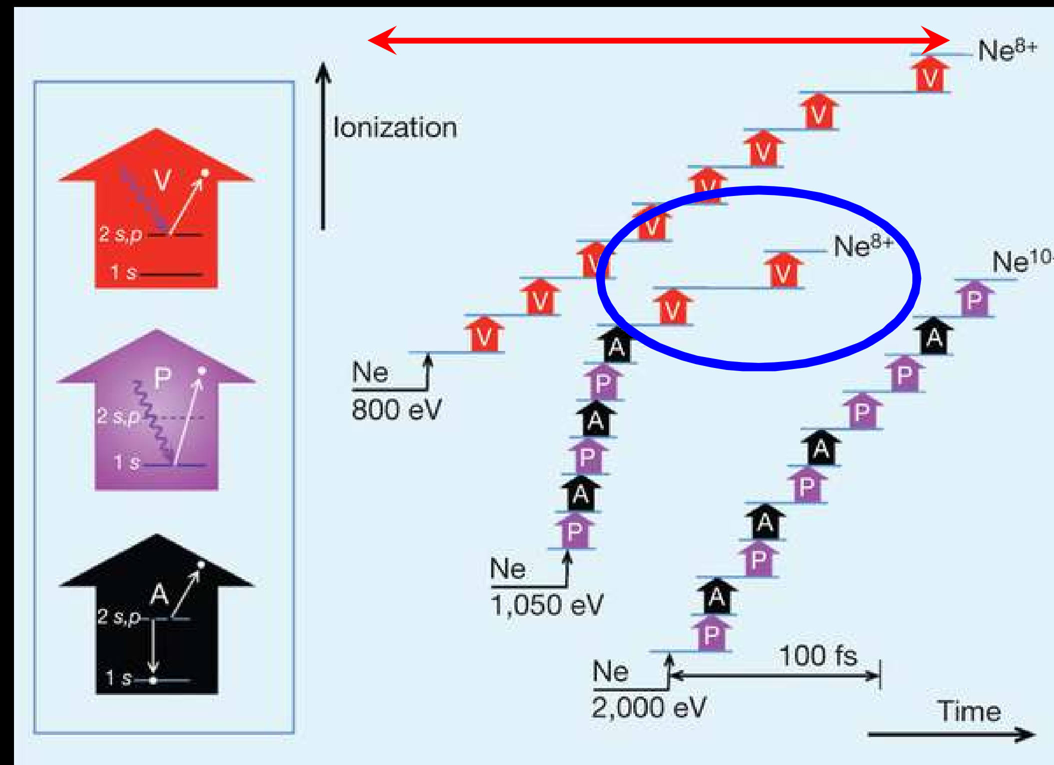
”Lav” fotonenergi: Neon 100% ioniseret på ~300 fs



Normal foto-ionisering

Kerne-elektron foto-ionisering

Auger-elektron henfald

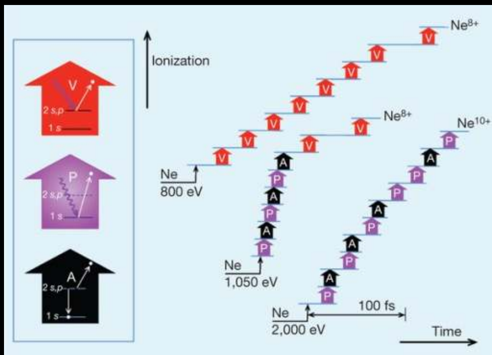


Højere fotonenergi, E= 1 keV
=> primært vekselvirkning med kerne-elektronerne:

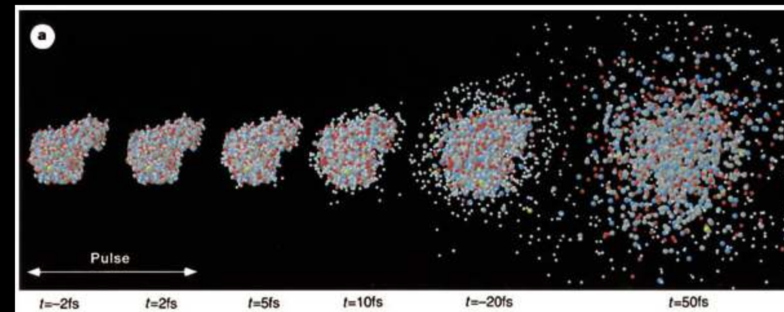
Neon^{8+} -ion med *kun* valenselektroner
(”Hollow neon”)

=> Ny viden om fundamental atomfysik og stof/strålingsvekselvirkninger

Molecular Movies



De ioniserede elektroner undslipper
=> Coulomb-eksplosion

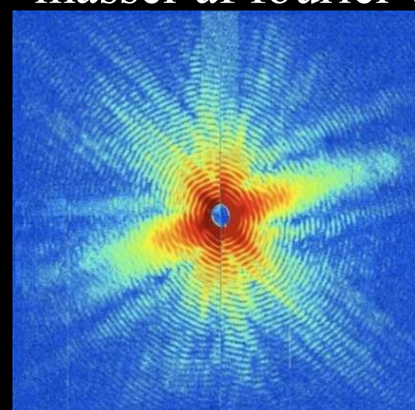


-på 10-50 fs, så med korte pulser kan man stadig måle strukturen
(”Diffract and Destroy”)

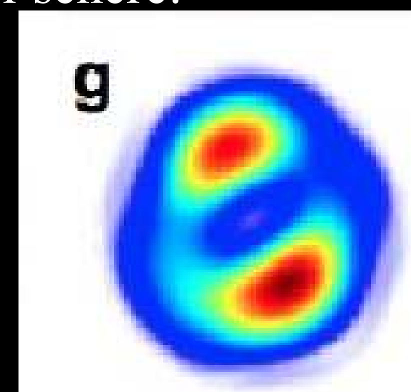
Enkelt-partikel billeddannelse
med ultrakorte pulser, mimi-virus:

200 nm

100.000+ billeder, snedig sortering og
masser af fourier-transformationer senere:

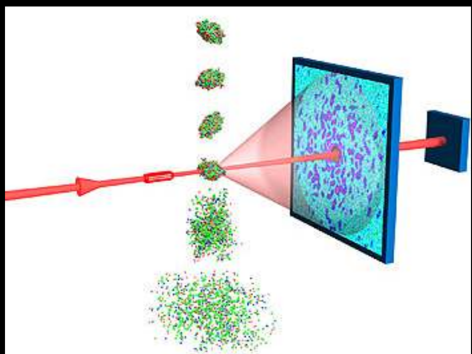


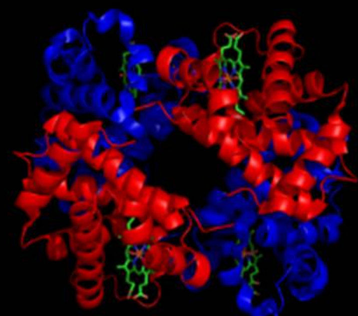
(Bemærk: ingen diffraktionspletter)



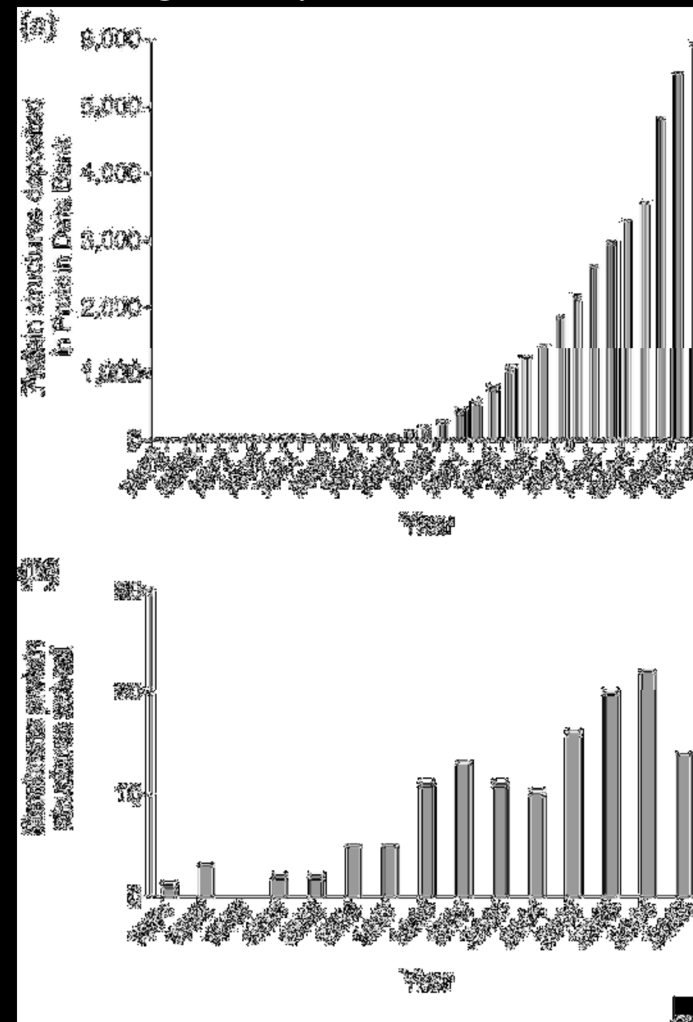
3D-struktur af virus-partikler

Målet for enkelt-partikel billeddannelse:
Enkelt-protein billeddannelse

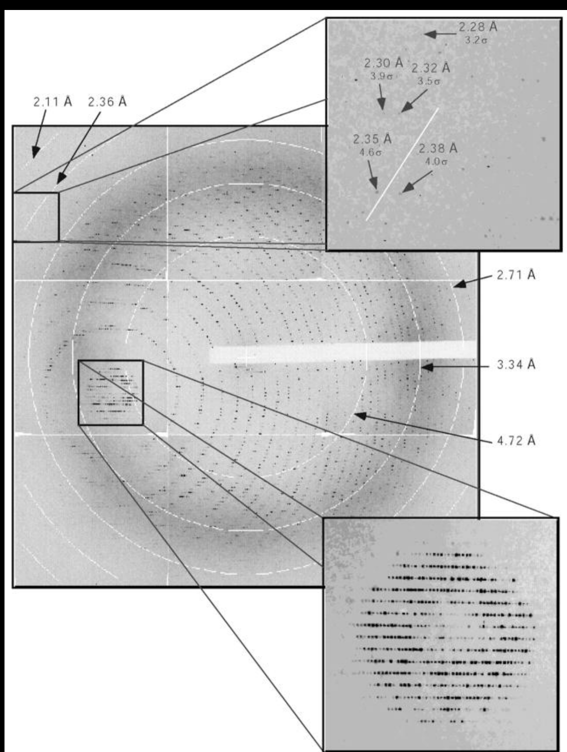


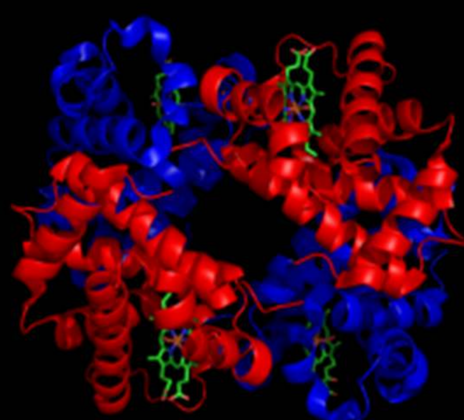


Men ikke alle proteiner kan ”nemt” krystalliseres...særligt membranproteiner er meget vanskelige at krystallisere



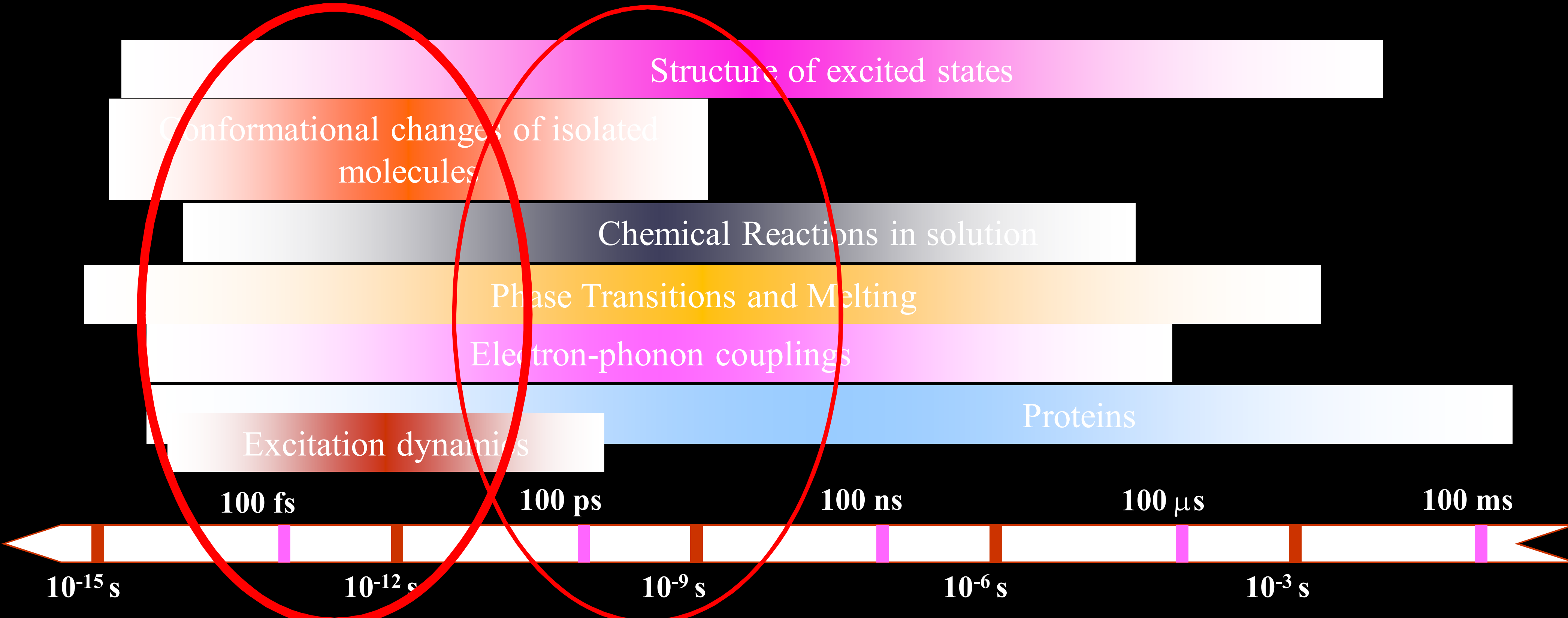
Protein-krystal diffraktion virker...
-så hvorfor?

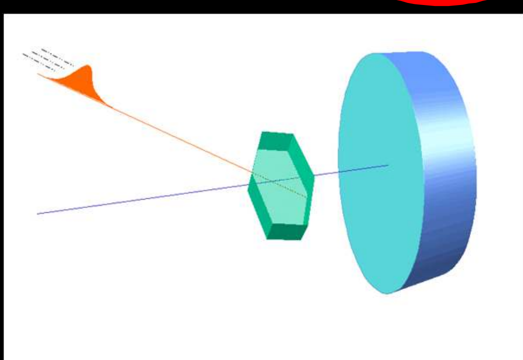




=> XFELs = ingen (store) krystaller =>*awesome* for strukturbiologi!

En anden herlig ting ved XFELs: De *Ultra*-korte røntgenpulser, < 100 fs

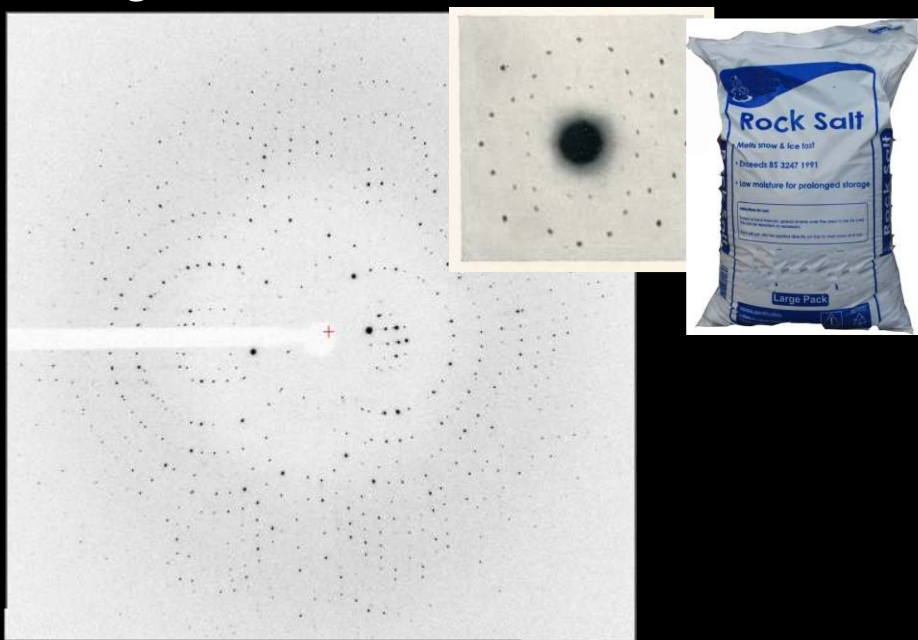


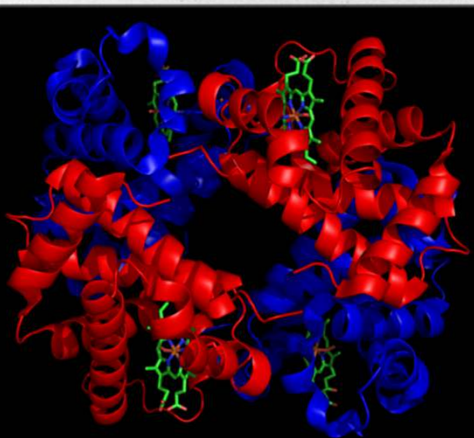


- Start with system in state A
- *Pump* system to state A* ⟵ UV-VIS-IR laser puls
- Wait Δt
- *Probe* the system in state A*
- Relaxation...
- *Repeat* for new Δt

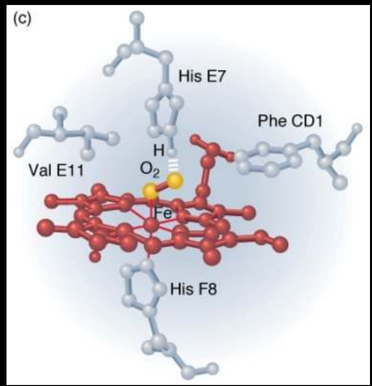
”Molecular Movies”

Røntgen er fantastisk til strukturbestemmelse

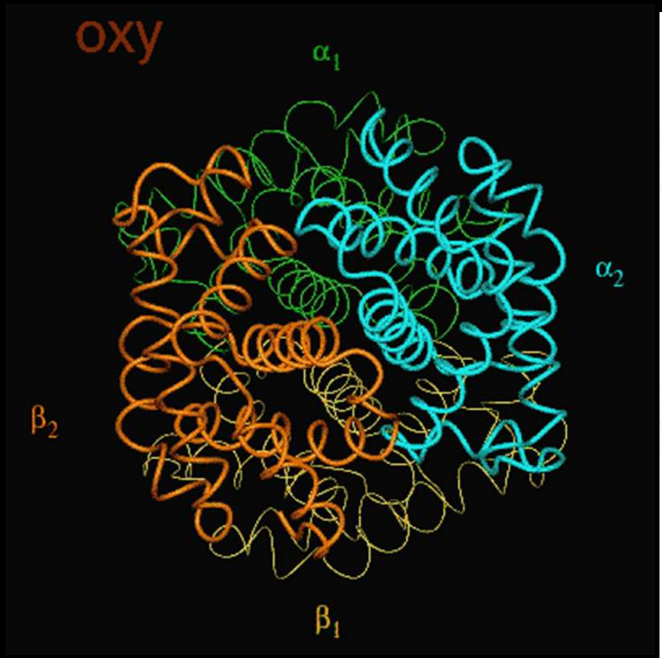




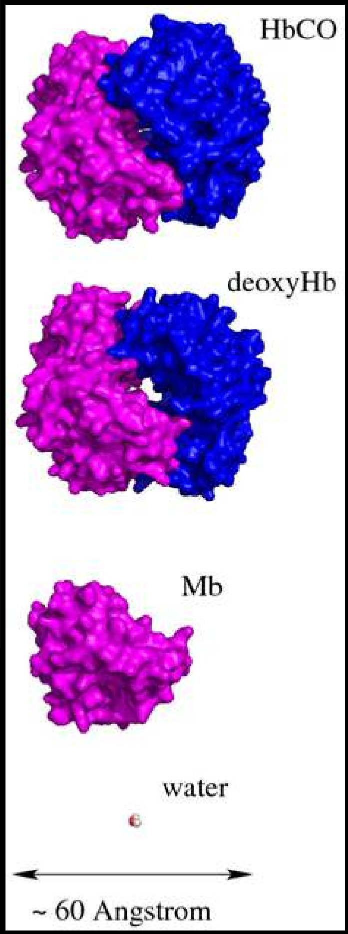
Hæmoglobin,
O_2/CO_2 transport



-Men strukturer forandrer sig....



Structural change -> many times higher affinity for binding O2



⇒ For at forstå funktionaliteten, må man forstå den *dynamiske* struktur

⇒ Og for at forstå den, må man kunne ”se” den

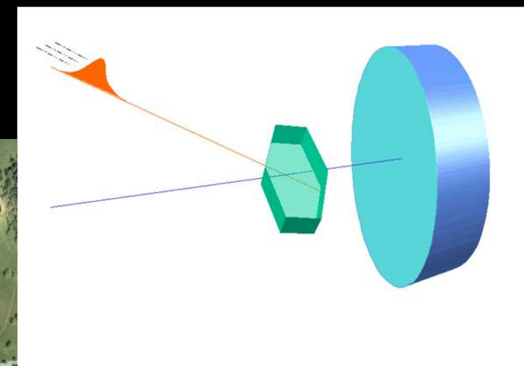
Why ultrafast?

Molecular Movies

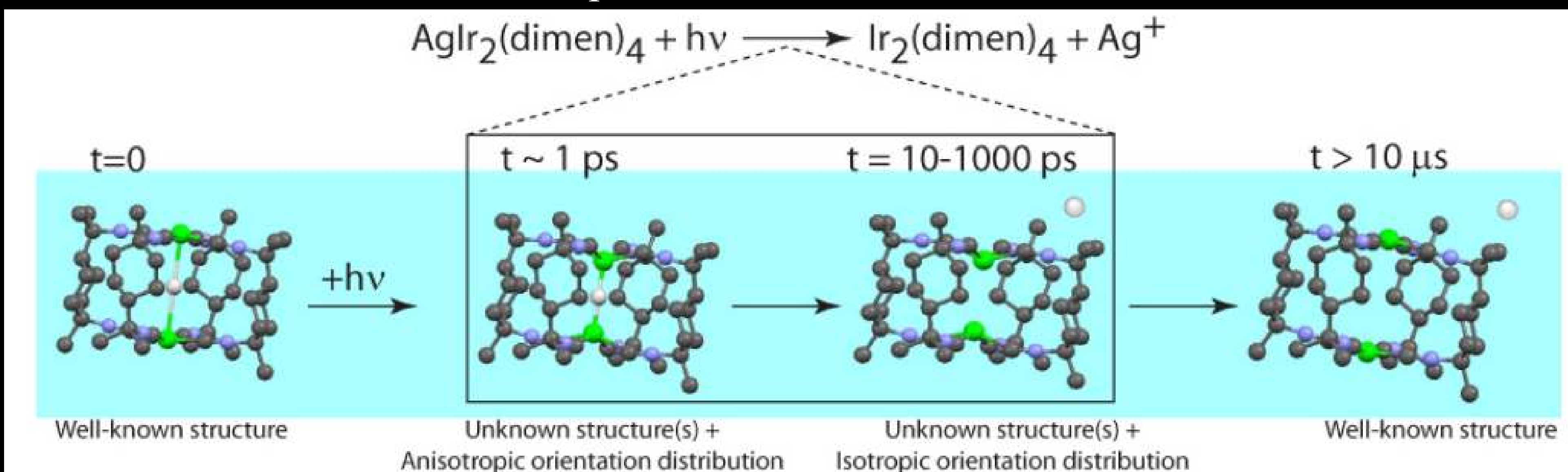
Et dybere blik ind i Kemien:

A + B ⟶ C

AB? BA?



Nu kan vi se ”ind i” reaktionspilen, som varer 1/1.000 af 1/1.000.000.000 sekund

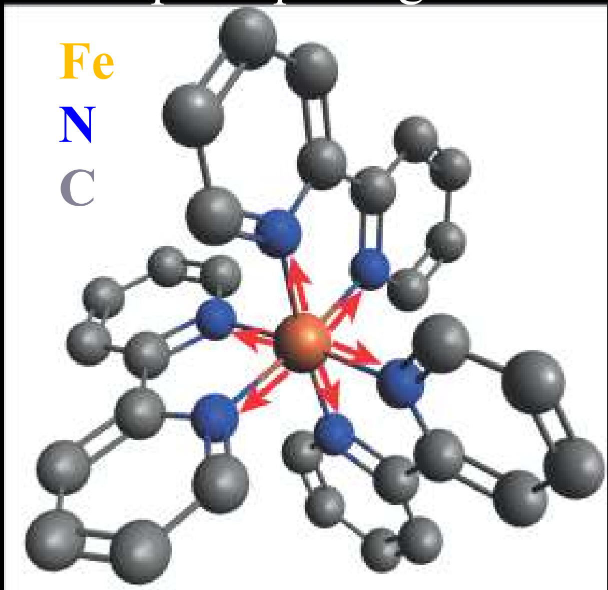


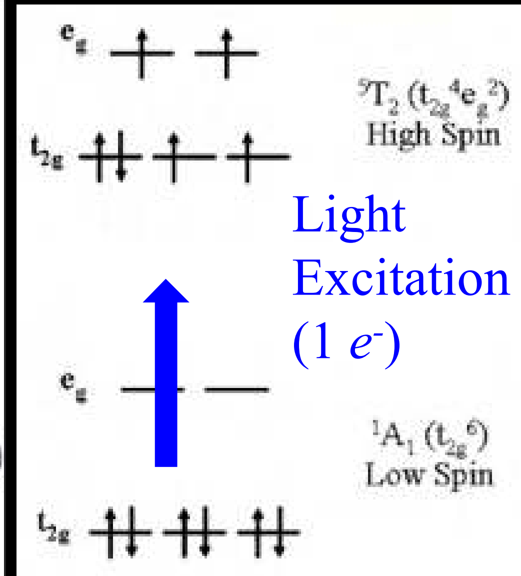
”The making&breaking of the chemical bond”

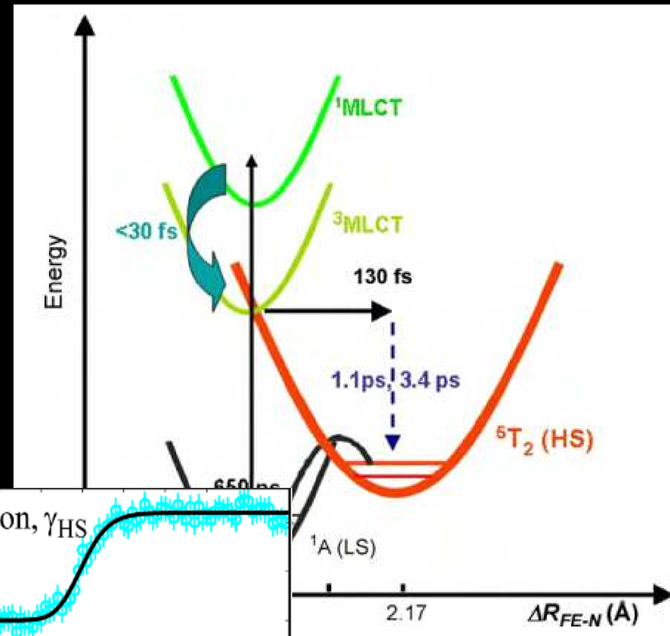
“Real-time studies of chemistry in action”

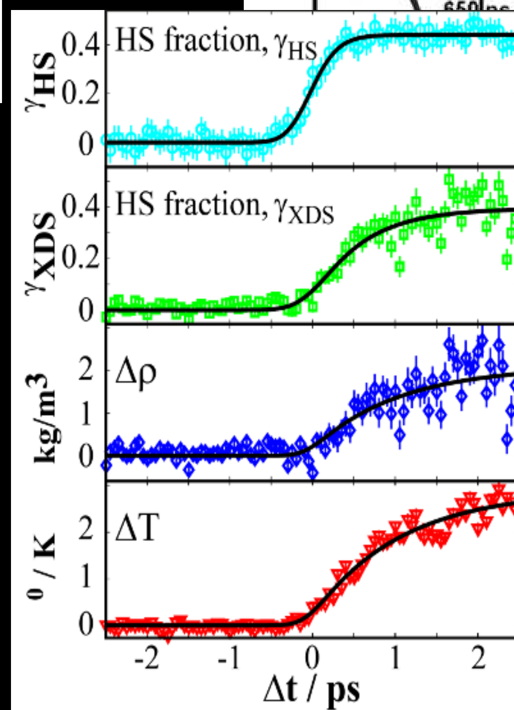
”Birth of a molecule”

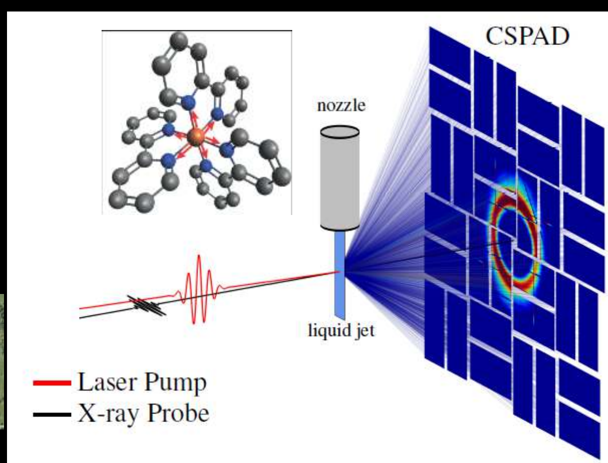
Eksempel: Spin- og strukturel dynamik i $Fe(bpy)_3$: Spin=0 til spin=2 ved at excitere een elektron







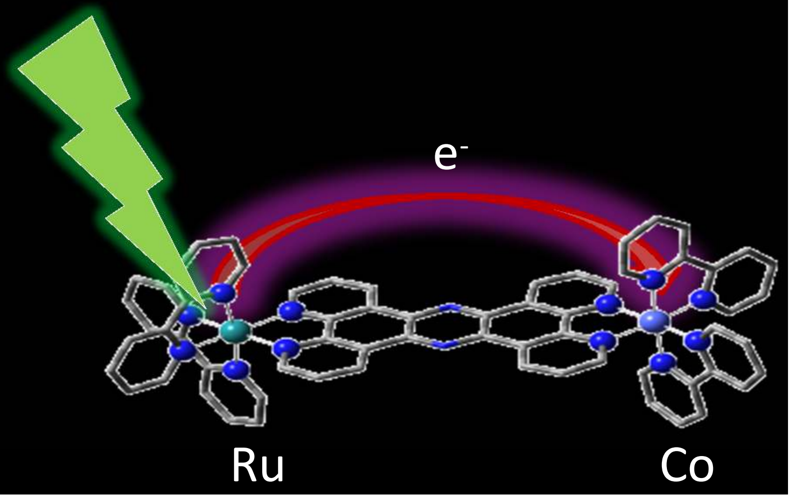


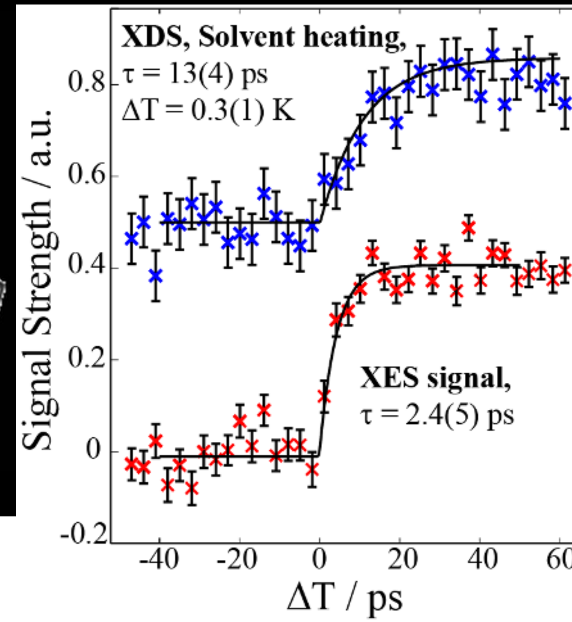


dT/dt ~ 10^{12} K/s

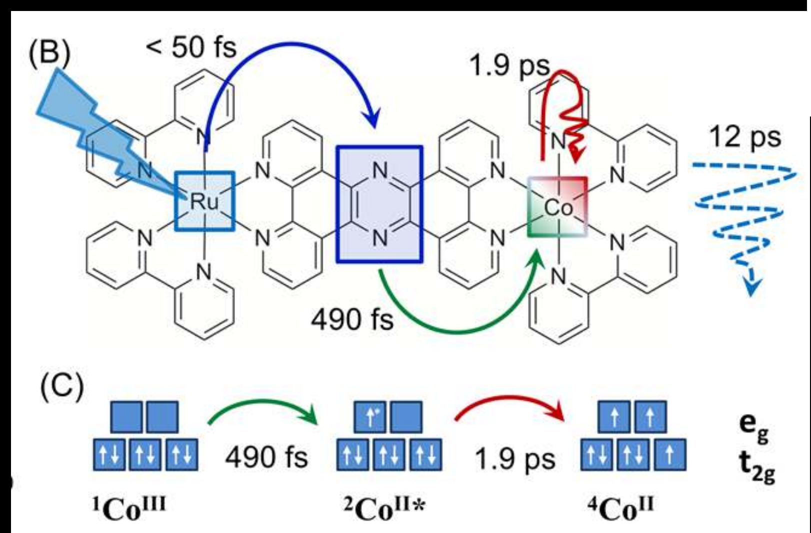
Movies in pre-production

Systems for solar energy conversion:





Our former students, now postdocs, Tim&Kasper. Along with the rest of us, among the first non-Japanese to carry out experiments at SACLA



~0.5 ps electron transfer time

~2 ps spin-state dynamics

~10 ps ”molecular cooling” time indicated by the solvent response

XFEL-anvendelser:

Fundamental atom/molekylefysik

Proteinstrukturer uden (store) krystaller

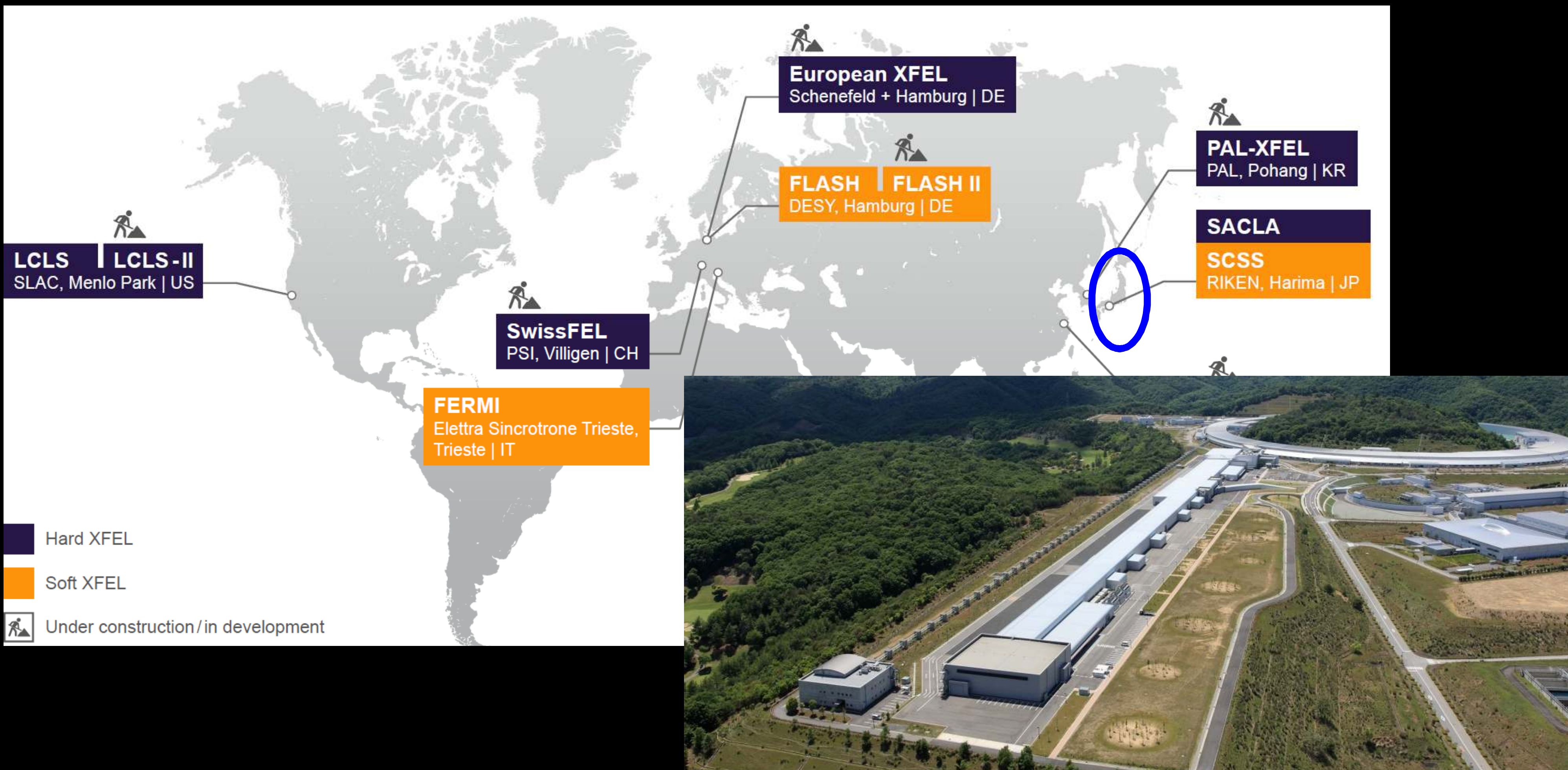
Studier af kemi og biologi med ultrahurtig tidsopløsning

Materialer under ekstreme forhold (geo-/planet- og bombe-fysik...)

-Og meget, meget mere!

⇒ Alle vil have en XFEL, nu!

DK er partner i det Europæiske XFEL-projekt, Euro-XFEL


European XFEL
Schenefeld + Hamburg | DE
FLASH
FLASH II
DESY, Hamburg | DE
PAL-XFEL
PAL, Pohang | KR
SACLA
SCSS
RIKEN, Harima | JP
LCLS
LCLS-II
SLAC, Menlo Park | US
SwissFEL
PSI, Villigen | CH
FERMI
Elettra Sincrotrone Trieste, Trieste | IT
Hard XFEL
Soft XFEL
Under construction / in development

Den Europæiske XFEL i Hamborg:

Project	LCLS US	SACLA Japan	European XFEL	SwissFEL Switzerland	PAL-XFEL Korea
Max. electron energy (GeV)	14.3	8.5	17.5	5.8	10
Wavelength range (nm)	0.13–4.4	0.06–0.3	0.05–4.7	0.1–7	0.06–10
Photons/pulse	~ 10^{12}	2 x 10^{11}	~ 10^{12}	~ 5 x 10^{11}	10^{11}–10^{13}
Peak brilliance	2 x 10^{33}	1 x 10^{33}	5 x 10^{33}	1 x 10^{33}	1.3 x 10^{33}
Pulses/second	120	60	27 000	100	60
Date of first beam	2009	2011	2016	2016	2015

The **European XFEL** (**X**-Ray **F**ree-**E**lectron **L**aser) is a research facility under construction which will provide high intensity X-ray light to help scientists better understand the nature of matter.

- Location: Schenefeld and Hamburg, Germany
- User facility with 260 staff (+230 from DESY)
- 2017 start of user operation

XFEL Financial participation (2005 Euro)

663 M€*

306 M€*

36 M€

33 M€

25 M€*

17.5 M€*

17 M€*

12.7 M€

11 M€

11 M€

11 M€

Denmark is a voting member, and the company *JJ X-ray* at DTU Scion is delivering the FXE instrument financed as an in-kind contribution

Molecular Movies

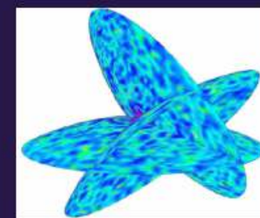
European XFEL

Enlightening Science

Scientific instruments:

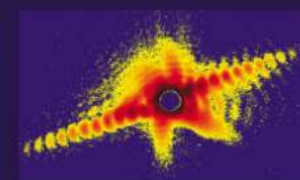
SPB: Ultrafast Coherent Diffraction Imaging of Single Particles, Clusters, and Biomolecules

Structure determination of single particles: atomic clusters, bio-molecules, virus particles, cells.



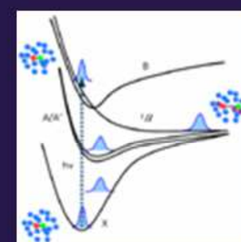
MID: Materials Imaging & Dynamics

Structure determination of nano-devices and dynamics at the nanoscale.



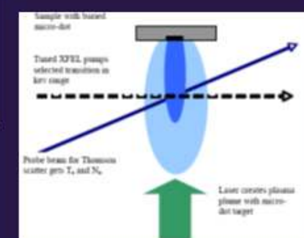
FXE: Femtosecond X-ray Experiments

Time-resolved investigations of the dynamics of solids, liquids, gases



HED: High Energy Density Matter

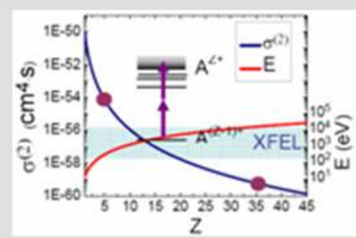
Investigation of matter under extreme conditions using hard X-ray FEL radiation, e.g. probing dense plasmas



Soft x-rays

SQS: Small Quantum Systems

Investigation of atoms, ions, molecules and clusters in intense fields and non-linear phenomena



SCS: Soft x-ray Coherent Scattering/Spectroscopy

Electronic and real structure, dynamics of nano-systems and of non-reproducible biological objects

Røntgen Fri-Elektron lasere, XFELs, er fantastiske maskiner:

10^6 mere intense end synkrotroner

Strålingen er koherent, hvilket tillader avanceret billeddannelse

Pulserne er <100 fs, 1000 * kortere end hidtil muligt

Den kraftigste XFEL i verden bliver bygget i Hamburg til 2017

Danmark er en partner i projektet

DTU-Fysik koordinerer leveringen af instrumentet til tidsopløste studier

Fremtiden er kun lige begyndt, og det tegner til at blive et vildt og underholdende ridt!

-Tak til jer, for jeres opmærksomhed!

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Molecular Movies

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Molecular Movies team, 2011-14

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